14.3.2 Organic analytical reagents used in NMR spectroscopy

Shift reagents

The term shift reagent is now almost synonymous with the paramagnetic lanthanide chelates, the most commonly used being complexes of europium(III) and praseodymium(III) with α -diketones. These complexes are Lewis acids and their action as shift reagents depends entirely on their ability to bind basic molecules (substrates) as labile ligands. Organic molecules that contain heteroatoms with a lone pair of electrons (oxygen, nitrogen, etc.) are potentially suitable substrates. The position of a given peak is related to the stability of the complex formed, the amount of shift reagent added, and the location of the observed nucleus relative to the lanthanide ion.

Relaxation reagents

Relaxation reagents are paramagnetic substances capable of strongly decreasing the relaxation times of substrate nuclei without inducing noticeable shifts. Both an electron-nuclear dipolar interaction and an electron-nuclear contact interaction may contribute to the overall relaxation.

Derivatizing reagents

They are used for tagging a molecule or functional moiety of interest via an appropriate derivative.